

ECE 371

Materials and Devices

08/27/19 - Lecture 2

The Crystal Structure of Solids

General Information

- Homework #1 assigned and due before class on Tuesday Sept 3rd
- Reading for next time: 2.1-2.2.1

Crystal Planes and Miller Indices

- Describe planes within the crystal using three integers (hkl) called Miller indices
- To find the Miller indices of a plane
 1. Find the intercept of the plane with the crystal axes and express those intercepts as a multiple of the basis vectors
 2. Take the reciprocals of the three numbers found in step 1
 3. Multiply by the lowest common denominator to obtain the smallest integers
 4. Replace negative integers with a bar over the number (i.e., $-h \rightarrow \bar{h}$)

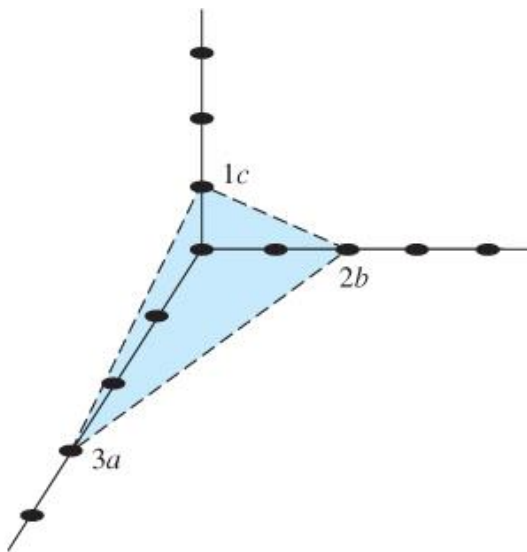


Figure 1.6 | A representative crystal-lattice plane.

The Miller indices of this plane are (236)

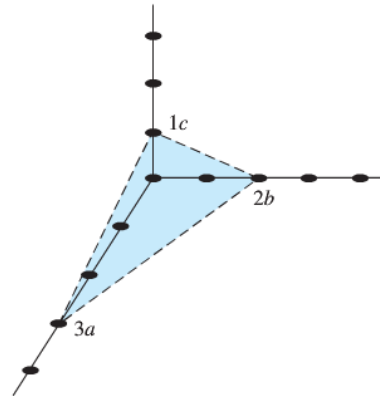
Notes:

- If a plane is parallel to an axis, we say it intercepts at ∞
- If a plane passes through the origin, it can be translated
- Individual planes are described with round brackets (hkl)
- Families of planes are described with curly brackets $\{hkl\}$

Crystal Planes and Miller Indices Example

EXAMPLE 1.2

Objective: Describe the plane shown in Figure 1.6. (The lattice points in Figure 1.6 are shown along the \bar{a} , \bar{b} , and \bar{c} axes only.)



*Miller indices define a set of parallel planes

Figure 1.6 | A representative crystal-lattice plane.

■ Solution

From Equation (1.1), the intercepts of the plane correspond to $p = 3$, $q = 2$, and $s = 1$. Now write the reciprocals of the intercepts, which gives

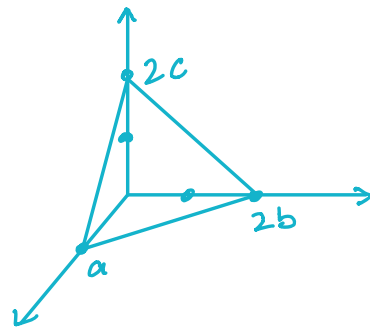
$$\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{1}\right)$$

Multiply by the lowest common denominator, which in this case is 6, to obtain (2, 3, 6). The plane in Figure 1.6 is then referred to as the (236) plane. The integers are referred to as the Miller indices. We will refer to a general plane as the (hkl) plane.

■ Comment

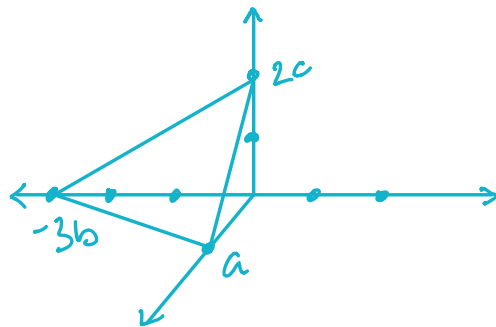
We can show that the same three Miller indices are obtained for any plane that is parallel to the one shown in Figure 1.6. Any parallel plane is entirely equivalent to any other.

Ex 1.7



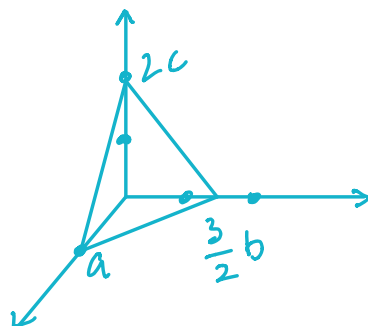
$$\begin{pmatrix} 1 & 2 & 2 \\ \frac{1}{1} & \frac{1}{2} & \frac{1}{2} \\ (2 & 1 & 1) \end{pmatrix}$$

Negative intercepts



$$\begin{pmatrix} 1 & -3 & 2 \\ \frac{1}{1} & -\frac{1}{3} & \frac{1}{2} \\ (6 & 2 & 3) \end{pmatrix}$$

In between intercepts



$$\begin{pmatrix} 1 & \frac{3}{2} & 2 \\ \frac{1}{1} & \frac{2}{3} & \frac{1}{2} \\ (6 & 4 & 3) \end{pmatrix}$$

Common Planes in Cubic Lattices

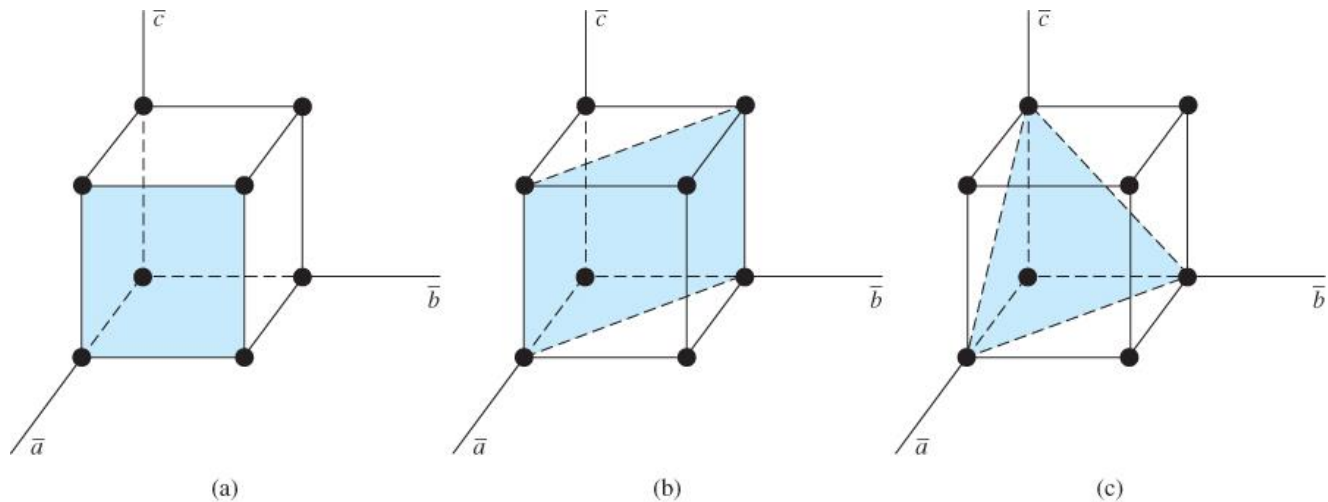


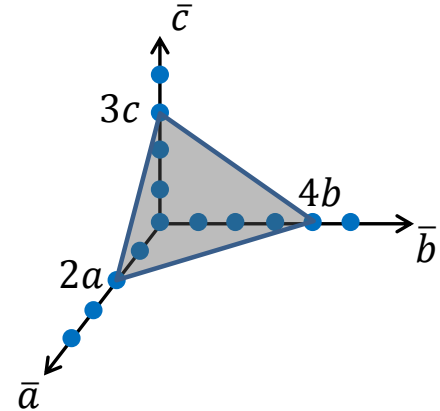
Figure 1.8 | Three lattice planes: (a) (100) plane, (b) (110) plane, (c) (111) plane.

- (100) silicon is the most common for modern transistors
- Bell Labs originally used (111) and Texas Instruments used (100)
- (111) has a higher atomic density (more dangling bonds), forms a weaker oxide, and has a more reactive surface, so (100) won out

Questions

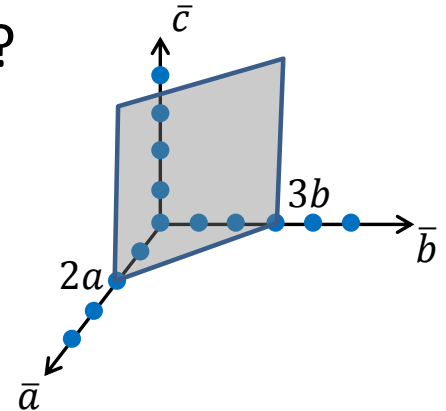
- What are the miller indices of this plane?

- A: (234)
- B: (634)
- C: $(\frac{1}{2} \frac{1}{4} \frac{1}{3})$
- D: (612)



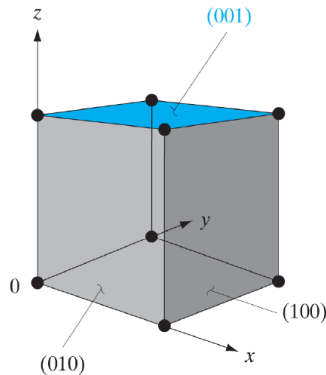
- What are the miller indices of this plane?

- A: $(\bar{2}30)$
- B: (461)
- C: (230)
- D: (320)



Equivalent Planes

- Planes may be translated or the choice of axes and origin may be changed to yield an equivalent “family” of planes, denoted by curly brackets $\{ \}$
- For example, in a cubic structure, the planes (100), (010), and (001) are crystallographically equivalent and are denoted by the family $\{100\}$



*from Streetman text

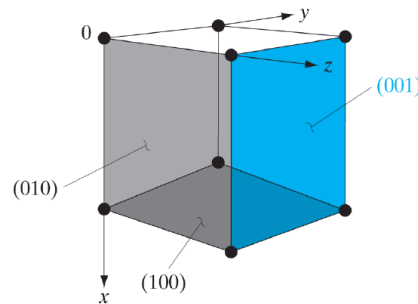


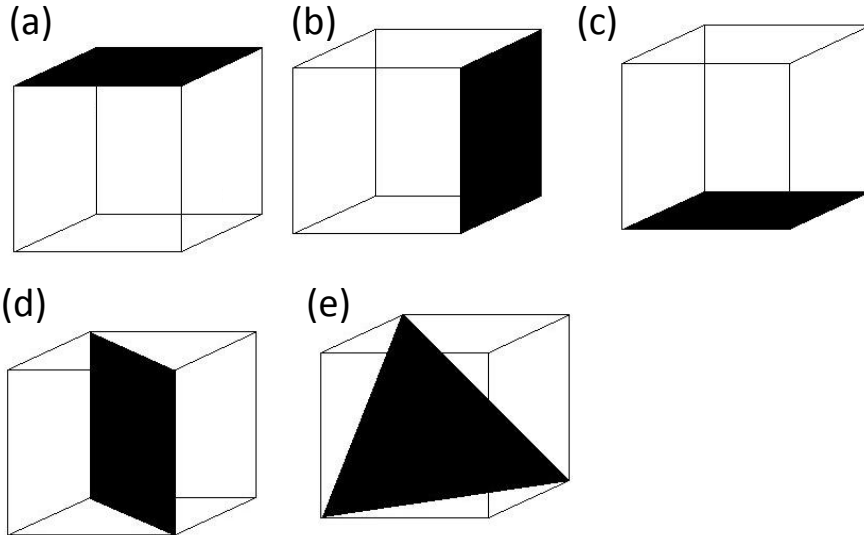
Figure 1.6

Equivalence of the cube faces ($\{100\}$ planes) by rotation of the unit cell within the cubic lattice.

Questions

- Which of the following planes could possibly be the $(10\bar{1})$ plane?

- A: (a)
- B: (b)
- C: (c)
- D: (d)
- E: (e)



- How many of these planes belong to the $\{100\}$ family?

- A: 1
- B: 2
- C: 3
- D: 4
- E: 5

Surface Density of Atoms

EXAMPLE 1.3

Objective: Calculate the surface density of atoms on a particular plane in a crystal.

Consider the body-centered cubic structure and the (110) plane shown in Figure 1.9a. Assume the atoms can be represented as hard spheres with the closest atoms touching each other. Assume the lattice constant is $a_1 = 5 \text{ \AA}$. Figure 1.9b shows how the atoms are cut by the (110) plane.

The atom at each corner is shared by four similar equivalent lattice planes, so each corner atom effectively contributes one-fourth of its area to this lattice plane as indicated in the figure. The four corner atoms then effectively contribute one atom to this lattice plane. The atom in the center is completely enclosed in the lattice plane. There is no other equivalent plane that

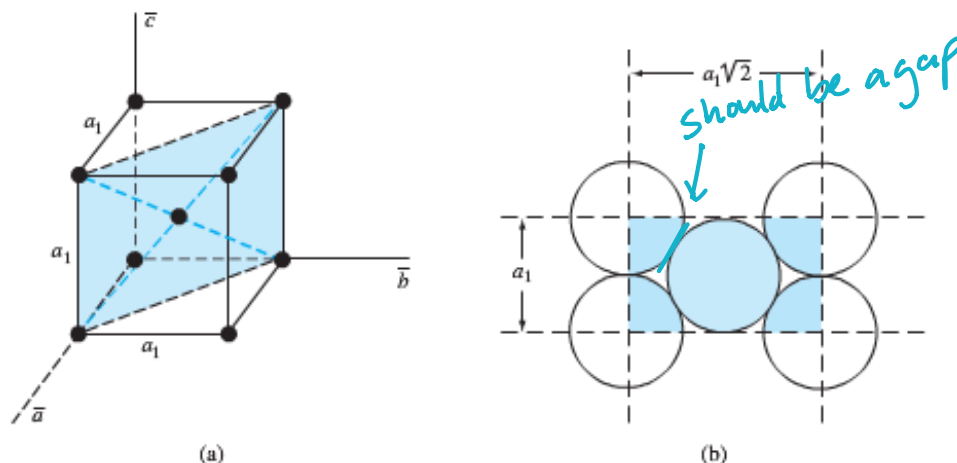


Figure 1.9 | (a) The (110) plane in a body-centered cubic and (b) the atoms cut by the (110) plane in a body-centered cubic.

Surface Density of Atoms

cuts the center atom and the corner atoms, so the entire center atom is included in the number of atoms in the crystal plane. The lattice plane in Figure 1.9b, then, contains two atoms.

■ Solution

The number of atoms per lattice plane is $\frac{1}{4} \times 4 + 1 = 2$

The surface density of atoms is then found as

$$\text{Surface Density} = \frac{\text{\# of atoms per lattice plane}}{\text{area of lattice plane}}$$

So

$$\begin{aligned} \text{Surface Density} &= \frac{2}{(a_1)(a_1\sqrt{2})} = \frac{2}{(5 \times 10^{-8})^2\sqrt{2}} \\ \text{SD} &= 5.66 \times 10^{14} \text{ atoms/cm}^2 \end{aligned}$$

■ Comment

The surface density of atoms is a function of the particular crystal plane in the lattice and generally varies from one crystal plane to another.

■ EXERCISE PROBLEM

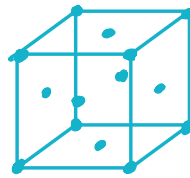
Ex 1.3 The lattice constant of a face-centered-cubic structure is 4.25 Å. Calculate the surface density of atoms for a (a) (100) plane and (b) (110) plane.

$$[\text{Ans. (a) } 1.11 \times 10^{15} \text{ cm}^{-2}; \text{ (b) } 7.83 \times 10^{14} \text{ cm}^{-2}]$$

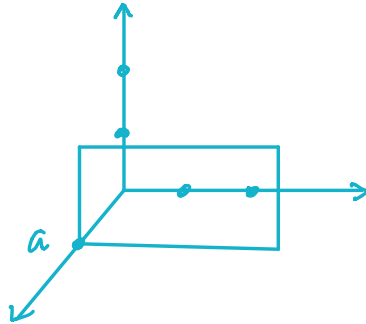
Ex 1.3

$$a = 4.25 \text{ \AA} = 4.25 \times 10^{-8} \text{ cm}$$

a) (100)



FCC = 2 atoms

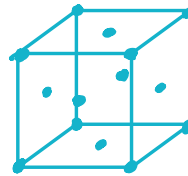


$$SD = \frac{\# \text{ atoms per plane}}{\text{area of plane}}$$

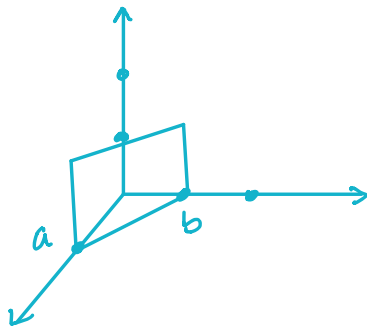
$$= \frac{2}{(4.25 \times 10^{-8})^2}$$

$$= 1.11 \times 10^{-5} \frac{\text{atom}}{\text{cm}^2}$$

b) (110)



FCC = 2 atoms



$$SD = \frac{\# \text{ atoms per plane}}{\text{area of plane}}$$

$$= \frac{2}{(4.25 \times 10^{-8})^2 \sqrt{2}}$$

$$= 7.83 \times 10^{-14} \frac{\text{atom}}{\text{cm}^2}$$

Directions in Crystals

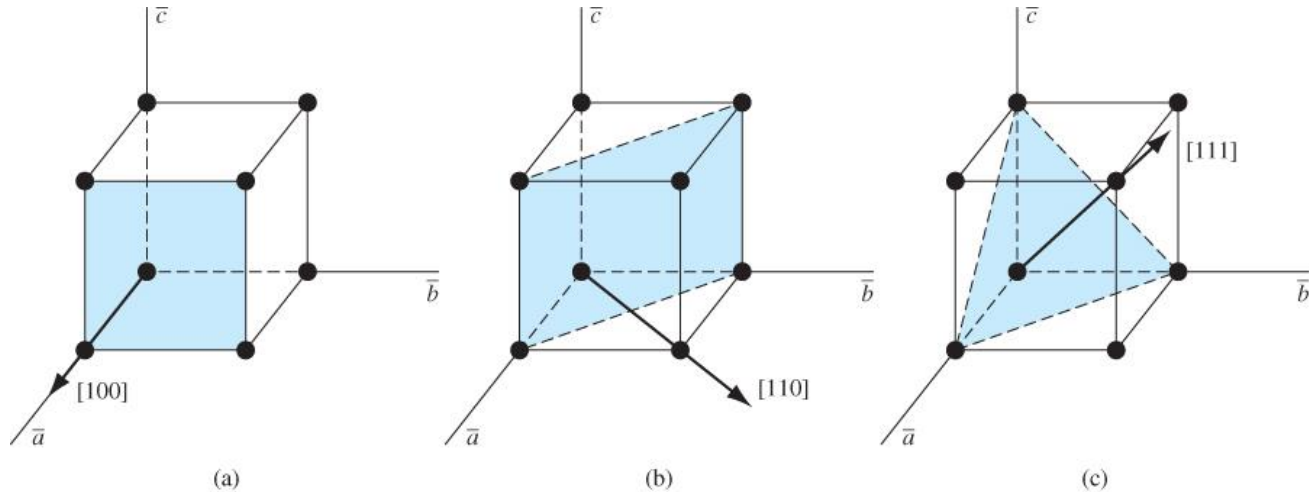


Figure 1.10 | Three lattice directions and planes: (a) (100) plane and [100] direction, (b) (110) plane and [110] direction, (c) (111) plane and [111] direction.

- Directions are represented with square brackets []
- A family of equivalent directions is given by pointy brackets $\langle \rangle$, (e.g., [100], [010], and [001] are all in the $\langle 100 \rangle$ family)
- For cubic lattices, the direction is perpendicular to the plane, but this is not necessarily true for other lattice structures (e.g., hexagonal)

*Is it possible to
create \perp directional
flow?
like diode*

The Diamond Structure

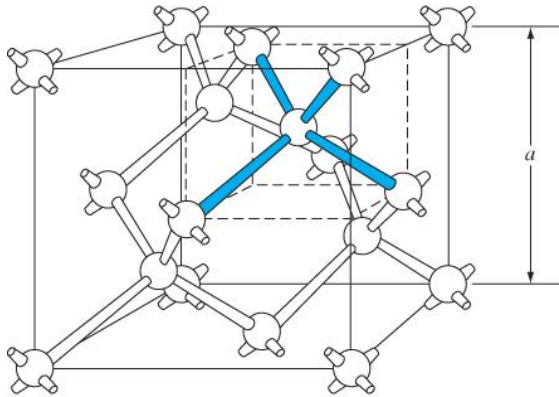


Figure 1.11 | The diamond structure.

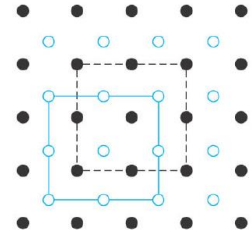
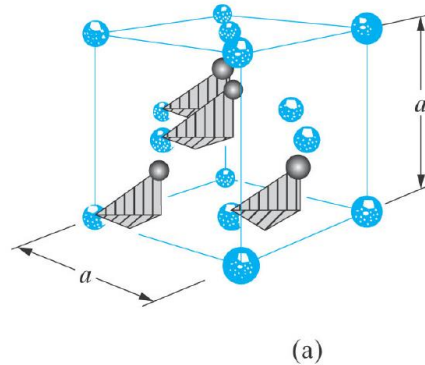
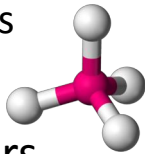


Figure 1.8

Diamond lattice structure: (a) a unit cell of the diamond lattice constructed by placing atoms $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from each atom in an fcc; (b) top view (along any $\langle 100 \rangle$ direction) of an extended diamond lattice. The colored circles indicate one fcc sublattice and the black circles indicate the interpenetrating fcc.

- **Lattice configuration for Si and Ge**
- FCC lattice with two atoms per lattice cite
 - One atom at $(0,0,0)$ and one at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, two interpenetrating FCC lattices
- Results in *4 extra atoms per unit cell* compared to FCC **8 total**
- Diamond lattice has tetrahedral bonding (i.e., four nearest neighbors, bond angles $\sim 109.5^\circ$)



The Zincblende Structure

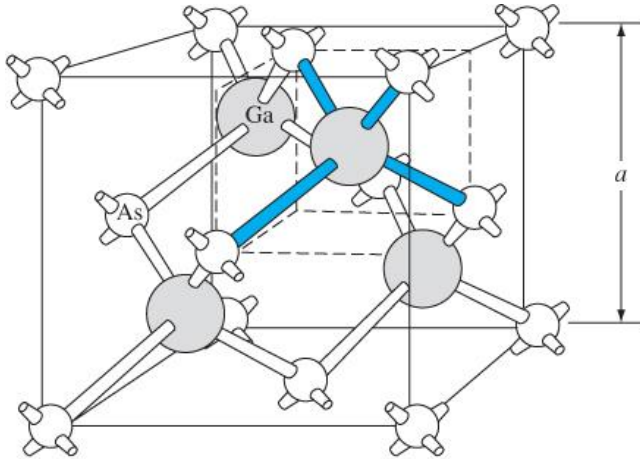
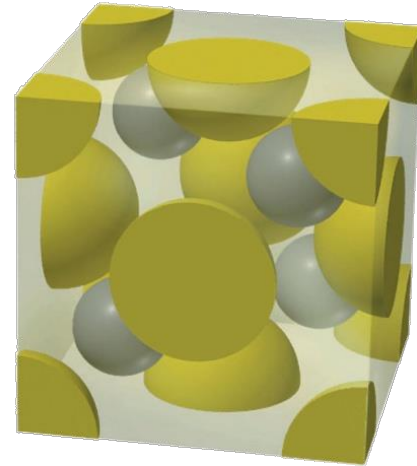


Figure 1.14 | The zincblende (sphalerite) lattice of GaAs.



- Same as diamond lattice, but the extra atoms at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ are of a different element
- Most compound semiconductors exhibit the zincblende structure (GaAs, InP, etc.)
- In GaAs, each Ga atom has four nearest neighbor As atoms

Bonding



Figure 1.16 | Representation of (a) hydrogen valence electrons and (b) covalent bonding in a hydrogen molecule.

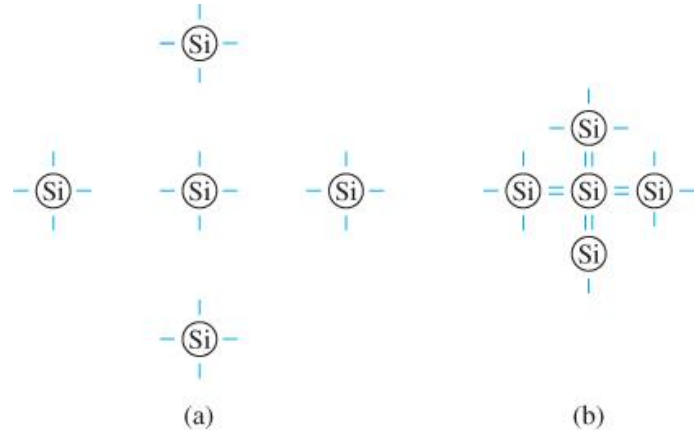
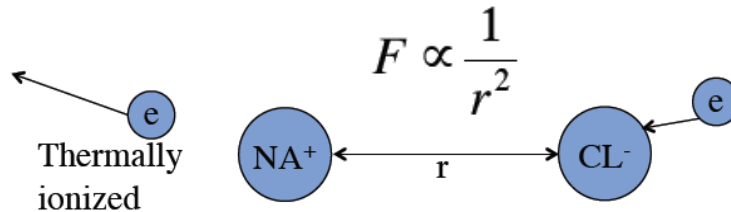


Figure 1.17 | Representation of (a) silicon valence electrons and (b) covalent bonding in the silicon crystal.

- Crystal finds lowest energy configuration
- Formation of complete valence shells
- Ionic bonding results in electrons being exchanged (e.g., NaCl)
- Covalent bonding results in electrons being “shared” (e.g., H₂)

Attractive vs. Repulsive Forces

- Attractive force: Coulomb force (e.g. - Na⁺ and Cl⁻)



- Bond formed with well defined atomic spacing (0.28 nm)
- *Why is spacing not zero?*
- Pauli exclusion principle:
 - States that no two identical fermions (e.g., electrons) may simultaneously occupy the same quantum state.
 - When two fermions with the same quantum states are brought together, they experience a repulsive force known as **Pauli repulsion**.

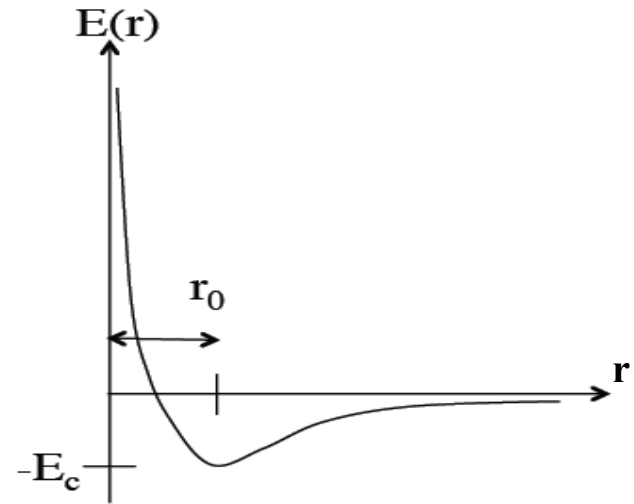
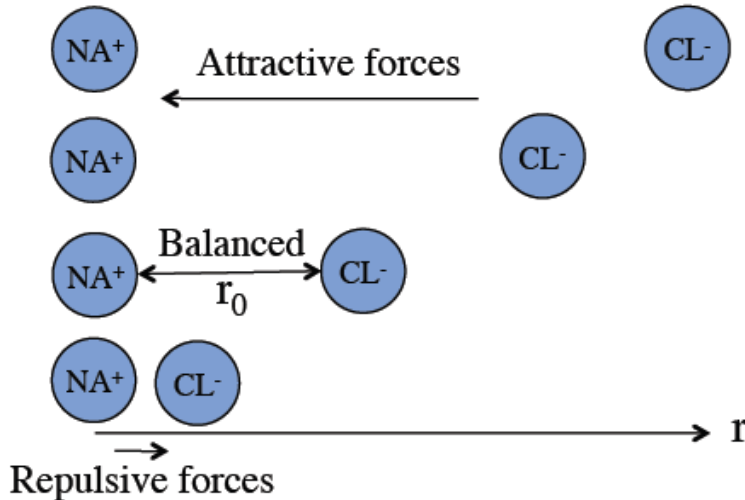
Qualitative Properties of Bonding

1. Energy tends to zero at large distances (zero energy in the absence of interaction)
2. At large distances energy is negative and increases with increasing distance. From infinity to r_0 the atoms are attracted to each other.
3. At very small distances, energy rises rapidly and atoms repel each other.
4. Curve has a minimum where attractive and repulsive forces balance each other.

We can use these properties to construct a curve of Energy vs. Separation

Energy vs. Distance

- At equilibrium, attractive forces and repulsive forces are balanced
- r_0 is the inter-atomic distance at equilibrium
- E_c is the bond energy (cohesive energy)



Defect Types

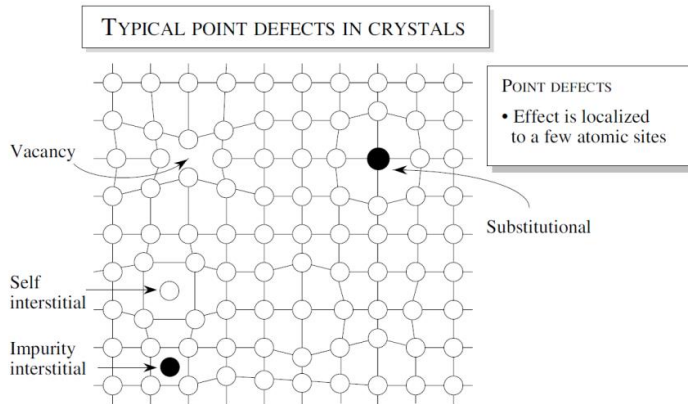


Figure 1.13: A schematic showing some important point defects in a crystal.

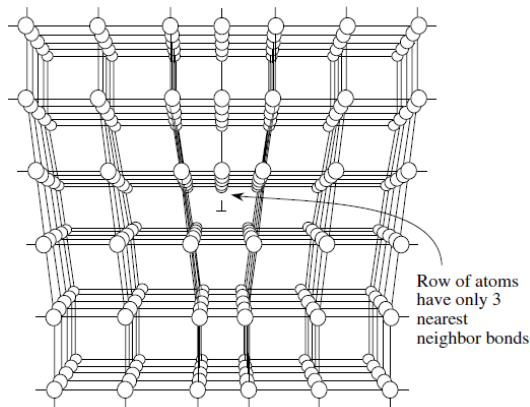
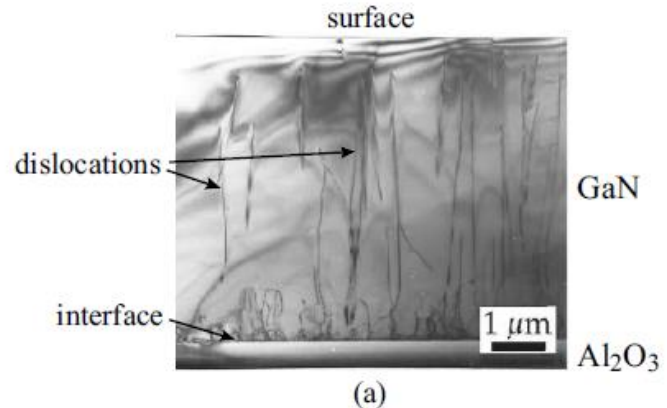


Figure 1.14: A schematic showing the presence of a dislocation. This line defect is produced by adding an extra half plane of atoms.

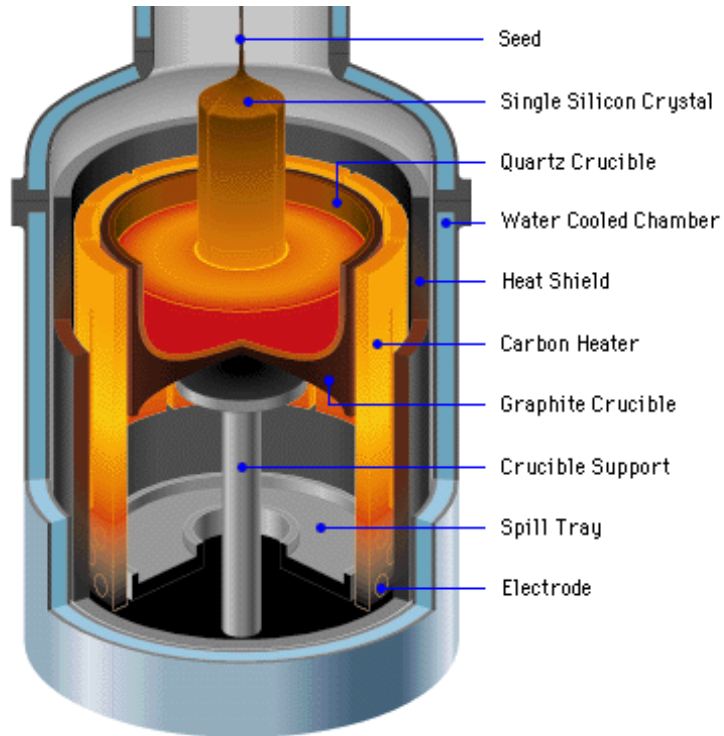
- Interstitials - *atom site b/t*
- Vacancies - *should be atom there*
- Antisite defects - *wrong atom in spot*
- Threading dislocations - *line of missing atoms*



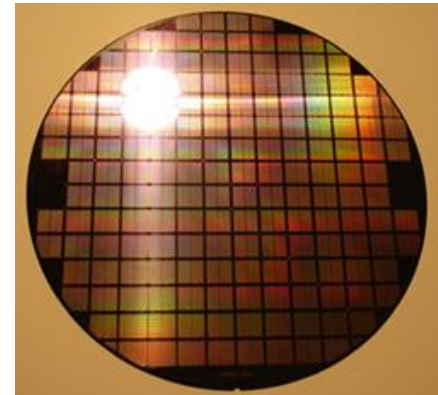
Mishra (2012)

Silicon Growth and Wafers

silicon boule growth

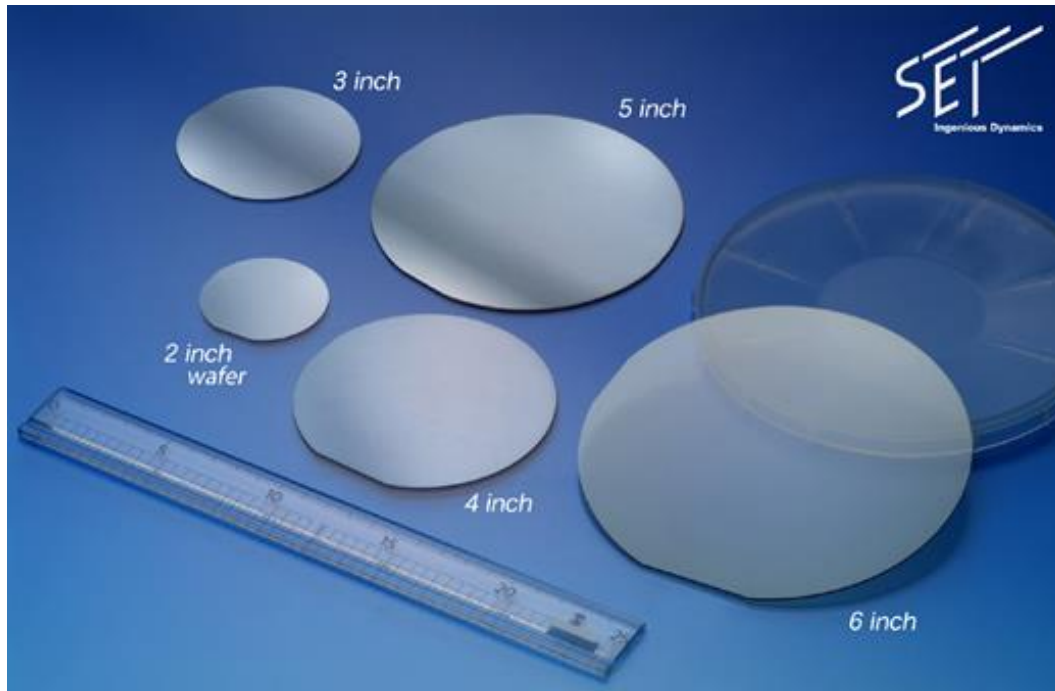


silicon boules and wafers



http://people.seas.harvard.edu/~jones/es154/lectures/lecture_2/materials/materials.html

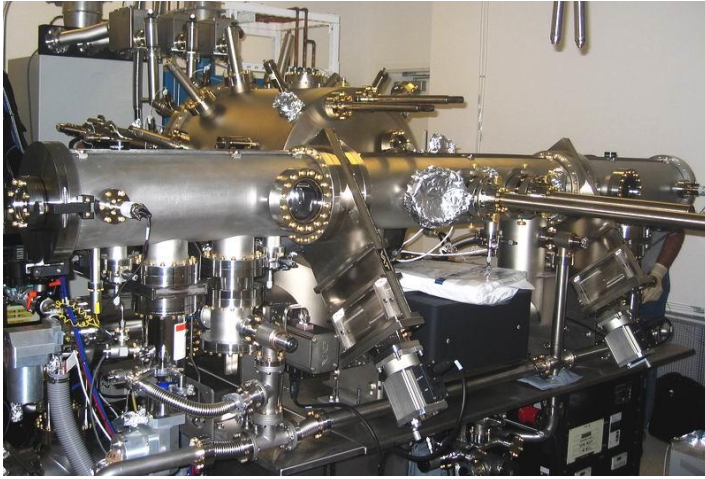
Substrates



source: http://www.semiconductor-today.com/news_items/2010/NOV/SEI_191110.htm

Epitaxy for III-V Materials

Molecular Beam Epitaxy (MBE)



- Research scale
- Ultra-high vacuum
- Lower temperature
- Abrupt interfaces
- Atomic layer control

Metal Organic Chemical Vapor Deposition (MOCVD)



- Production scale (high growth rate)
- Close to atmospheric pressure
- Higher temperature
- High quality layers
- Difficult to monitor growth rate
- Toxic gases needed

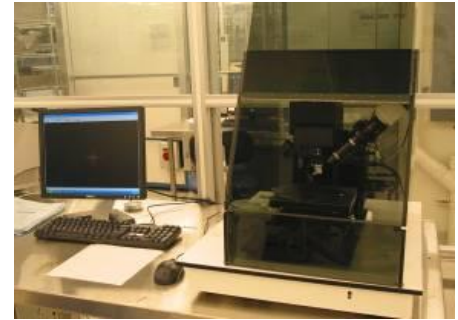
Front-End Fabrication



Photolithography



Wet processing



Metrology



Thin film deposition



Thermal processing



Dry processing